

Abstract Submitted
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Charge Localization and near zero in-plane thermal expansion in layered Na_xCoO_2 , $x \sim \frac{1}{2}$ DIMITRI ARGYRIOU, C. MILNE, O. PROKHENKO, Hahn-Meitner-Institut, Glienicker Str. 100, Berlin D-14109, Germany, L.C. CHAPON, P.G. RADAELLI, ISIS Facility, Rutherford Appleton Laboratory-CCLRC,U.K. — We have used neutron powder diffraction and X-ray single crystal diffraction to investigate the lattice response to charge localization and magnetic ordering in samples with stoichiometry close to $\text{Na}_{0.5}\text{CoO}_2$ over the temperature range of 2 to 600K. Our measurements show there presence of two crystallographical distinguishable Co sites but with essentially identical bond valences. This indicates only a marginal charge disproportionation between Co^3 and Co^4 . Our measurements show Na-ordering achieved by de-intercalation imposes a constraint on the charge and spin-state degrees of freedom that acts as to reduce the in-plane thermal expansion to near zero values between 2 to 300K. At higher temperatures we find a phase non-reversible transition to a phase with a $3a \times 3b \times c$ cell, wtr to the orthorhombic $Pnmm$ low temperature phase. This phase does not exhibit any of the anomalies observed at 52 and 87K in the magnetic susceptibility of the as made phase.

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